

DESIGN OF NANOMACHINES USING NANOENGINEER-1

John M. Espinosa-Duran, Jaime Velasco-Medina

Grupo de Bio-nanoelectrónica, EIEE. Universidad del Valle. A. A. 25360, Cali, Colombia

E-mail: {michaele, jvelasco} @univalle.edu.co

ABSTRACT

This article describes a basic design methodology for nanomachines using Nanoengineer-1, which is a molecular dynamic simulation software that allows to simulate nanomechanical events. This work presents the design of some nanomachines and the simulation of some nanomachines designed by Erick Drexler, which are oriented to be part of nanofactories and nanorobots. The simulation results show that nanoengineer-1 is a suitable software to design of nanomachines on a personal computer.

1. INTRODUCTION

In recent years nanotechnology has become one of the most important and exciting forefront fields in Physics, Chemistry, Engineering and Biology. It shows great promise for providing, us in the near future, any breakthroughs that will change the direction of technological advances in a wide range of applications [1].

The nanotechnology is being applied in many fields: to sense the neural activity [2], to clean up the spacecraft water [3], to deliver drug to a specific part of the body [4], to construct nanomanipulators [5], to improve the harvest [6], and to built electronic devices [7].

Many people are designing systems based in molecular dynamics and quantum theory rules, like nanodevices (sensors, transistors), nanomachines (motors, bearings, actuators), nanostructures (polymers, superconducting, composites) using computer simulations.

The complexity of: the quantum theory, the molecular dynamics and the modeling of systems using the Finite Elements Method (FEM) and the interaction between the elements (vibrational analysis) made difficult the design of nanomachines, therefore the simulations were executed on super-computers or massive parallel computer systems, available only in huge universities or companies and generally these simulations taken hours or days. However, using nanoengineer-1 these problems have been solved, because this allows to simulate nanomachines on a personal computer in minutes or hours (depending of the number of atoms).

This software is based on the idea of Erick Drexler of manipulating atom by atom in order to build nanosystems.

This work describes a basic design methodology for nanomachines using Nanoengineer-1 and presents the design of some nanomachines and the simulation of some nanomachines designed by Erick Drexler, which are oriented to be part of nanofactories and nanorobots.

This article is not oriented to describe the theoretical concepts about nanomechanical or nanothermodynamical, the objective is to motive the research community in this topic.

This work is organized as follows. Initially, section 2 describes the general features of Nanoengineer-1. In section 3, the basic principles of mechanosynthesis are presented. In section 4, a brief description of the design methodology for nanostructures is presented. In section 5, some considerations for simulation of nanomachines are presented. In section 6, some designs and simulation of nanomachines are presented. Finally, section 7 presents the conclusions and the future work.

2. NANOENGINEER -1: A NANOMECHANICAL SIMULATION TOOL

NanoENGINEER-1 is the first molecular 3D CAD program developed exclusively for nanomechanical engineering (see Figure 1), that includes both a sophisticated CAD module for the design and modeling of atomically precise components and assemblies, and a molecular dynamics module for setting up and simulating mechanical nanodevices to analyze motion, stiffness and other important design properties.

Nanoengineer-1 manages the following type of files: Protein DataBank (pdb), Molecular Machine Parts (mmp), Gamess (out), and it includes tools that allows to build highly symmetrical molecular structures, a simulator, a library with molecular gears, bearings, shafts, etc., and the following chemical elements: Hydrogen(H), Helium(He), Boron(B), Carbon(C), Nitrogen(N), Oxygen(O), Flourine(F), Neon(Ne), Aluminum(Al), Silicon(Si), Phosphorous(P), Sulfur(S), Chlorine(Cl), Argon(Ar), Germanium(Ge), Arsenic(As), Selenium(Se), Bromine(Br), Krypton(Kr) [8].

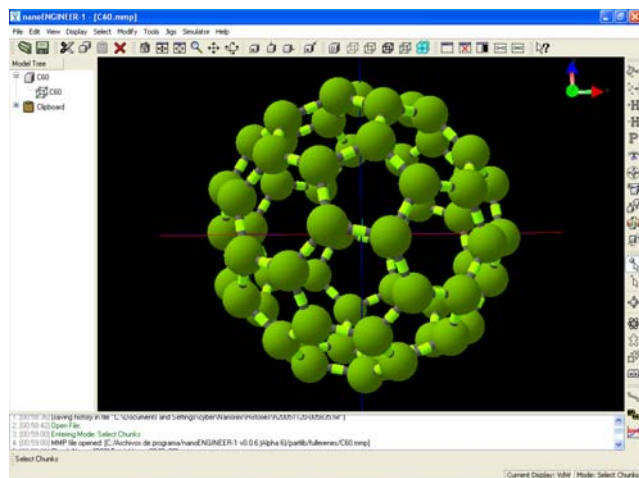


Figure 1. Nanoengineer -1 User Interface

3. BASIC PRINCIPLES OF MECHANOSYNTHESIS

Molecular NanoTechnology (MNT) is the projected ability to use nanotechnology for "molecular manufacturing", a proposed technology based on positionally-controlled mechanosynthesis guided by molecular machine systems. MNT would involve combining physical principles demonstrated by chemistry, other nanotechnologies, and the molecular machinery of life with the systems engineering principles found in modern macroscale factories. Its most well-known exposition is in the books of K. Eric Drexler. Formulating a roadmap for its development is now an objective of a broadly based technology roadmap project led by Battelle (the manager of several U.S. National Laboratories) and the Foresight Institute [9].

In conventional chemical synthesis or chemosynthesis, reactive molecules encounter one another through random thermal motion in a liquid or vapor. In a hypothesized process of mechanosynthesis, suggested notably by K. Eric Drexler [10], reactive molecules would be attached to molecular mechanical systems, and their encounters would result from mechanical motions bringing them together in planned sequences, positions, and orientations. It is envisioned that mechanosynthesis would avoid unwanted reactions by keeping potential reactants apart, and would strongly favor desired reactions by holding reactants together in optimal orientations for many molecular vibration cycles. Mechanosynthetic systems would be designed to resemble some biological mechanisms.

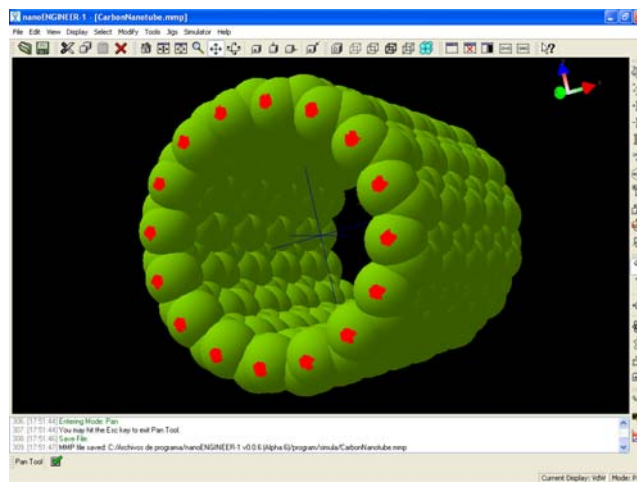
While the description of mechanosynthesis given above has not yet been achieved, primitive mechanochemistry has been performed at cryogenic temperatures using scanning tunneling scraping electron microscopes. So far, such devices provide the closest approach to fabrication tools for molecular engineering.

The mechanosynthesis will be fundamental to molecular manufacturing based on nanofactories capable of building

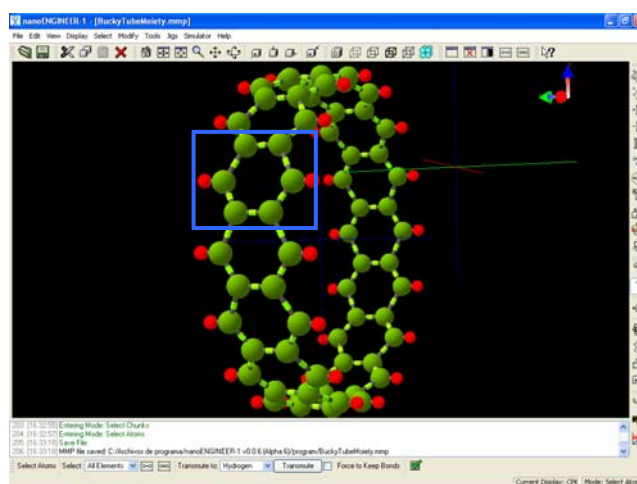
macroscopic objects with atomic precision and that is the basic idea of Nanoengineer-1 tool: design the machines that will be part of the nanofactory [10].

4. BASIC DESIGN METHODOLOGY FOR NANOSTRUCTURES

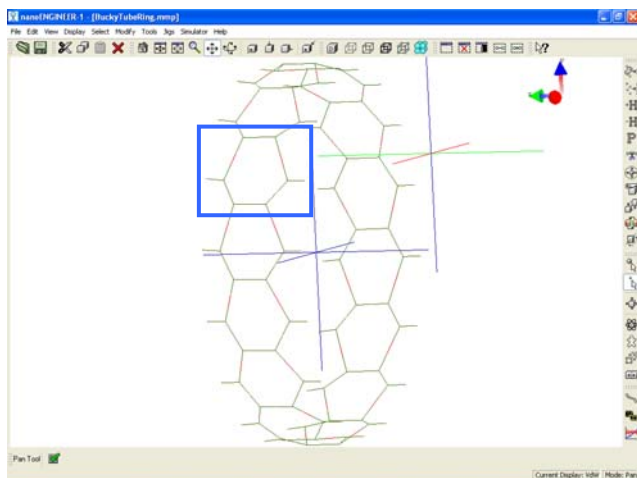
A basic methodology is described for designing of nanodevices (with symmetric structure) using nanoengineer-1. In order to understand it, a simple example is considered. In this case, the objective is to design a Carbon Nanotube (CNT) (see Figure 2a). Figure 2b shows the ring structure that is repeated along the nanotube. Figure 2c shows the basic crystallographic cell, which is repeated through the nanotube determining its structure. This cell is also formed by a moiety (see Figure 2d).



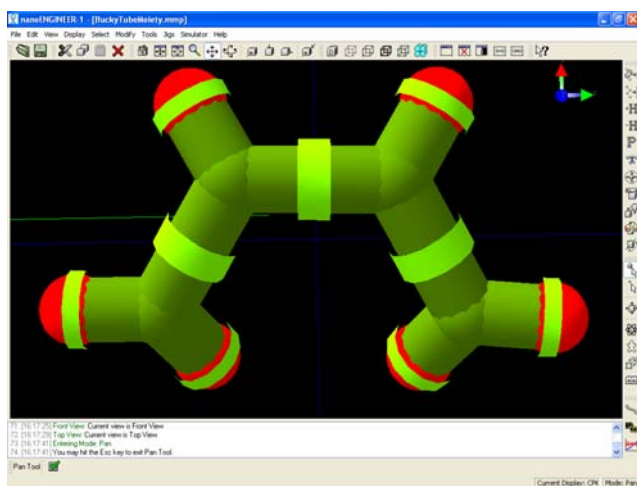
a)



b)



c)





d)

Figure 2. Design of a carbon Nanotube, a) carbon nanotube designed in *VdW* display mode, b) ring structure of the CNT in *CPK* display mode, c) basic crystallographic cell of the CNT in *Lines* display mode, d) basic moiety in *Tubes* display mode

4.1 Basic design methodology

The basic design methodology for symmetrical nanostructures is:

1. Determine the basic moiety (see Figure 2c).
2. Design the moiety by hand.
 - 2.1 Click the *build atoms* icon , which display a window with the available atoms.
 - 2.2 Select the appropriated atoms, Carbon (C) for the nanotube.
 - 2.3 Bond the atoms in the correct crystallographic orientation by drag-and-drop.
3. Extrude the basic moiety to obtain a complex structure
 - 3.1 Click the *extrude* icon , which shows other two moieties. The extrude tool allows to repeat automatically the moiety in rod or ring shape according to the available bonds.

- 3.2 Build the basic crystallographic cell (see Figure 2c) determining the bonds between the moieties, by dragging and dropping one of the moieties in the direction of the other. It will cause a change of color in the bonds that are going to carry out.
- 3.3 Extrude the moieties in ring shape using 16 moieties by selecting *ring* in the list of extrude mode, and writing *16* in the filed N. It allows to obtain the result showed in Figure 2b.
4. Extrude the last result (the complex ring structure) in the rod shape using 5 structures, in order to obtain the nanotube (see Figure 2a).

It is possible to design complex structures starting from simple ones because nanoengineer-1 allows to import designs.

It is necessary to take in account the basic chemistry of the design, for example the type of bond (simple, double, triple or aromatic), the spin level of the bond (sp , sp^2 , sp^3 in the case of the carbon), the real distances (a 3D grapheme structure has separation between each film) and other aspects.

5. RELEVANT ASPECTS ABOUT SIMULATION

For the nanomechanical simulation of the nanostructures it is possible to use a variety of elements, which are: Rotational motor, Linear motor, Ground, Thermostat, Thermometer and Gamess:

5.1 Rotational motor.

In the design of nanomachines for the future nanofactory this could be the most used. It emulates the behavior of a nanomotor that generates a torque to the nanomachine. To use it, first select the atoms where it will be attached, then select the *jig* menu, *rotational motor* option, and Figure 3 window will be displayed, which allows to introduce the parameters that determine the behavior of the motor: the name, the torque, the rotation speed, motor length, motor radius and spoke radius. Finally, click in OK. In this case, it is necessary to take in account the correct positioning of the motor because it could cause a bad-function or the destruction of the design.

5.2 Linear motor.

It is used to move a nanostructure in a linear direction. To use it, select the atoms to be moved and then select this jig, a window similar to Figure 3 is displayed which allows to introduce the parameters that determine the behavior of the motor: Force, Stiffness, Motor length, Motor width and Spoke radius. Then click in OK.

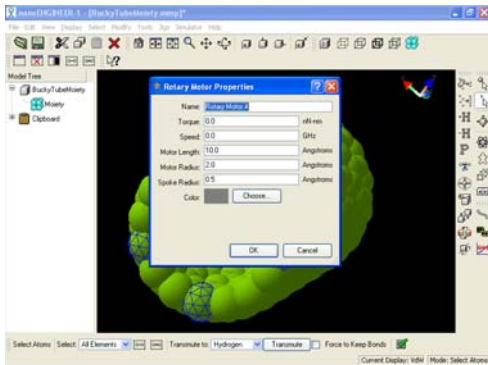


Figure 3. Rotational motor configuration window

5.3 Ground.

The ground determines the points (atoms) of the structure that are attached (fixed) to some rigid body, which does not allow to move freely the nanomachine. To use it, it is necessary to select first the atoms to be grounded and then select this in the *jig* menu.

5.4 Thermostat.

This element allows to measure the energy added to the nanostructure in a specific part. To use it, select the atom where the measure will be realized and then select this in the *jig* menu.

5.5 Thermometer

This element is used to measure the temperature in a specific part of the design. To use it, select the atom where the measure will be realized and then select this in the *jig* menu.

5.6 Gamess.

This jig is generally used by the chemical engineers.

After the simulation, Nanoengineer -1 generates a playback video, observable through its movieplayer, that shows the vibration and motion of the atoms of the design. To observed the values of the torque (generated by the motor and the induced in the ground), the force, energy added to the system (see figure 4) and temperature in a specific point, Nanoengineer -1 has a plot tool which allows to see, in a X-Y plane, the numerical values and a text file containing all the graphical information.

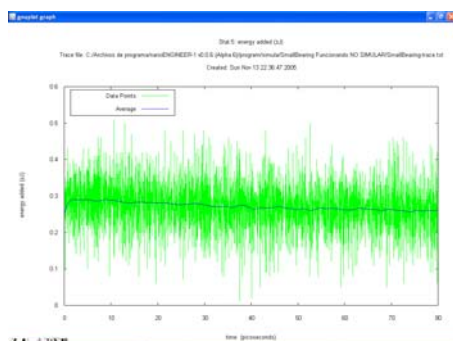


Figure 4. Plot of the energy added to a Bearing, measured by a thermostat during the simulation

When the design is finished and ready to simulate, the simulator displays a window to introduce the time of the simulation in frames, the time of each frame (in units of 0.1 femtoseconds), and the room temperature during the simulation.

6. DESIGNING WITH NANOENGINEER-1

This section presents the simulation of some designs of K. Erick Drexler and designs based on other works, which have application in building nanofactories or nanorobots.

6.1 Big Bearing.

The Big bearing showed in Figure 5, one of the classical designs of Drexler [11], is made of H, C, O, N and S, and it is implemented using a casing fixed to the ground and an inner sleeve that is attached to the motor. The motor was configured using the following parameters: torque 200nN-nm, speed 2000 GHz (These values are extreme, and were used to produce an interesting simulation as quickly as possible. A serious nanoengineer assessing the operating conditions of this bearing would have used more reasonable numbers), length 10Å, radio 2Å, and spoke radio 0.5Å. The simulator was configured for 2000 frames, with 200 steps per frame at 300°K. This design has 2808 atoms and 23 grounds.

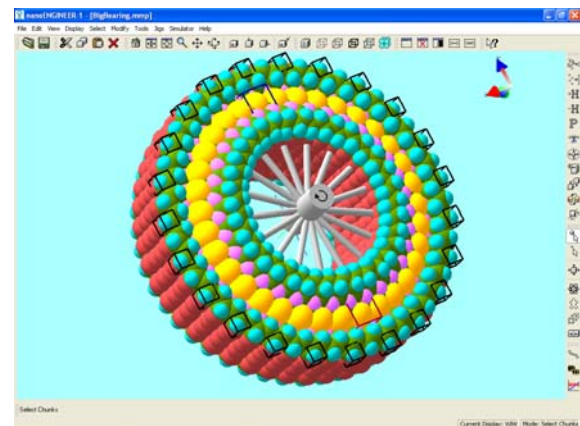
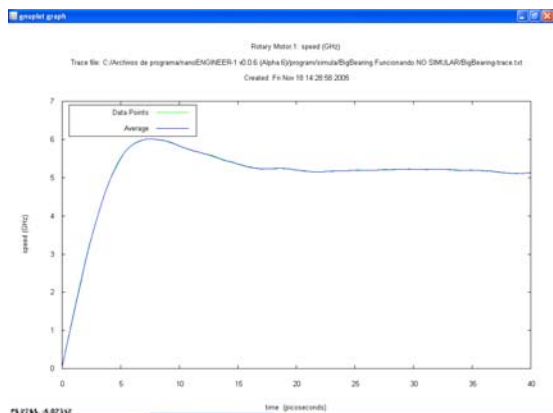
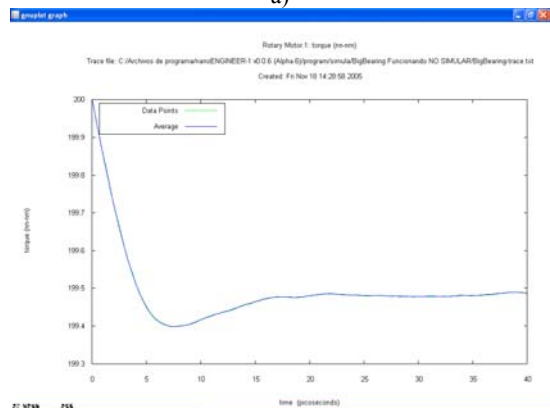


Figure 5. Drexler's Big Bearing using Nanoengineer -1

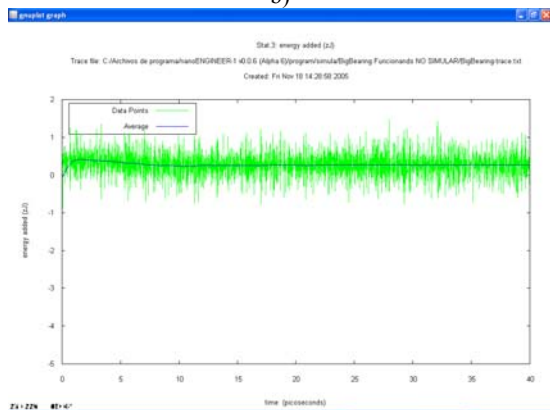
The simulation results (video) show that the big bearing turns 1 time. Figure 6a, shows the rotation speed of the motor which presents a similar behavior to a standard DC motor (it is saturated); it shows that in 40ps it achieves approximately 5GHz. Figure 6b shows the torque exerted by the motor, Figure 6c shows the energy added to the atom identified by + in Figure 5, Figure 6d shows the temperature measured on the atom identified by * in Figure 5, which vary a little due the friction between atoms during the turn and Figure 6e shows the torque exerted on the grounds, which vary due the vibration of the atoms and the force applied by the motor to the internal wall of the bearing case. In this case the variation of the variables measured is minimal due this structure is very stable.



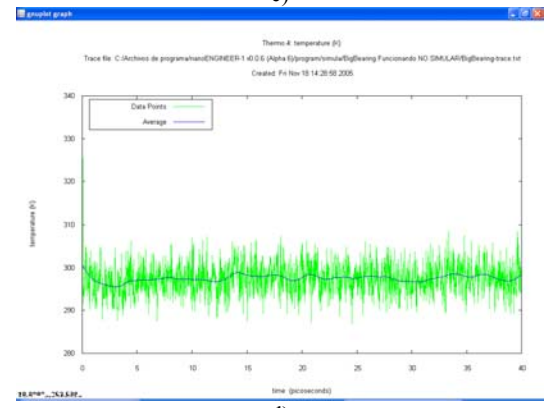
a)



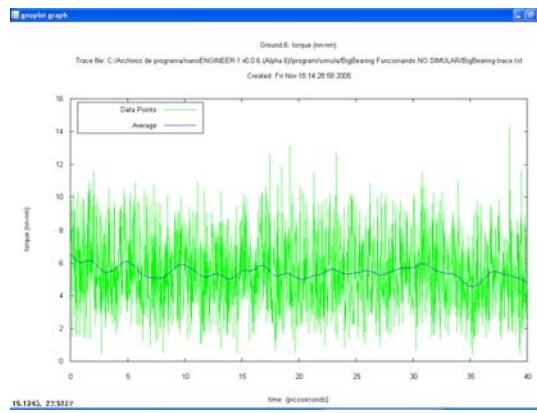
b)



c)



d)



e)

Figure 6. Graphical simulation results of the small bearing. a) Speed, b) Torque, c) Energy added, d) Temperature and e) Torque at the ground

6.2 LilGears Variation.

This gear is based on “LilGears” from the Nanoengineer-1 library, which is basically a pair of coupled motor-gears trying to rotate at different speeds. The new design proposed in this work is just one gear coupled to one motor as shows Figure 7. The gear is made C, O and N. The motor was configured using the following parameters: torque 20nN-nm, speed 2000GHz (2 THz), length 10Å, radio 2Å, and spoke radio 0.5Å. The simulator was configured for 1000 frames, with 200 steps per frame (20ps) at 300°K. This design has 170 atoms and 0 grounds (the upper cube is a thermostat and the under cube is a thermometer).

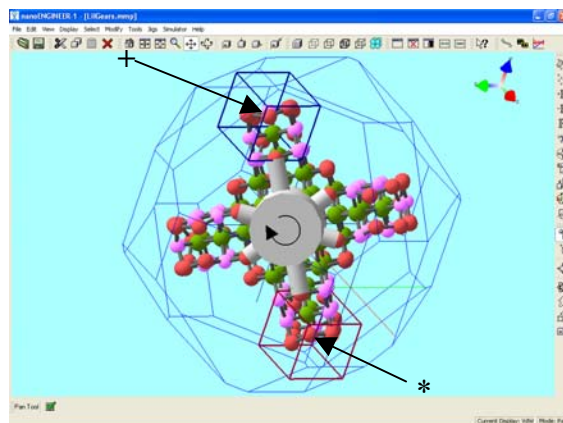
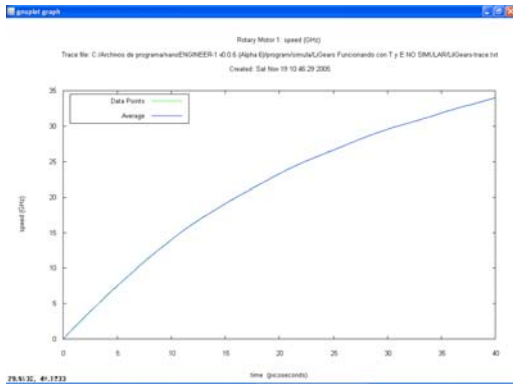
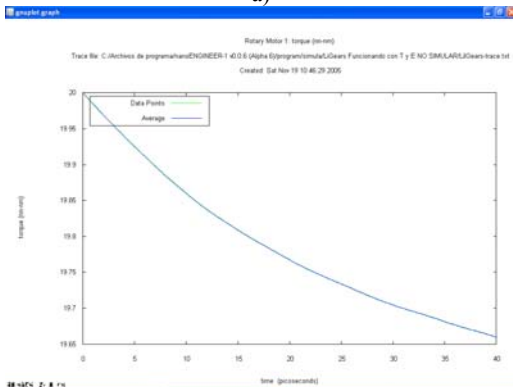


Figure 7. A stand alone Gear in CPK display mode, ready to simulate whit the chunk selected

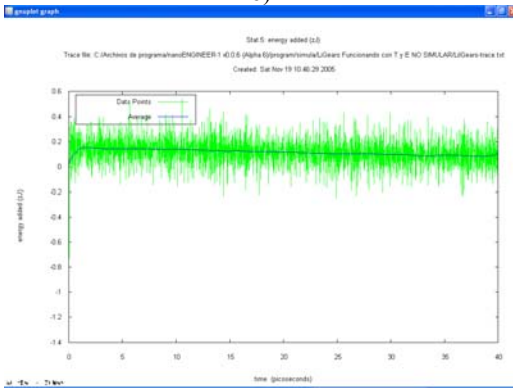
The simulation results (video) show that the gear turns 1 time. Figure 8a, shows the rotation speed of the motor growing exponentially; it shows that in 40ps it achieves approximately 34GHz, with growing tendency . Figure 8b shows the torque exerted by the motor, Figure 8c shows the energy added to the atom identified by + in Figure 7, Figure 8d shows the temperature measured on the atom identified by * in Figure 7.



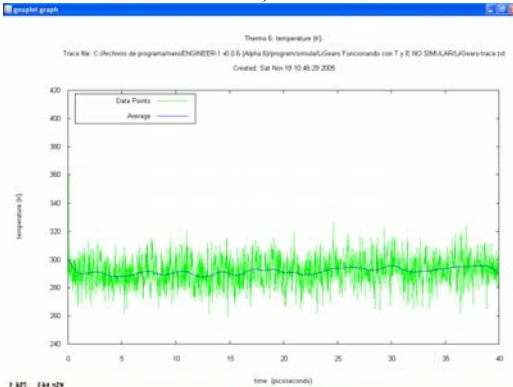
a)



b)



c)



d)

Figure 8. Graphical simulation results of the LilGears Variation.
a) Speed, b) Torque, c) Energy added, d) Temperature

Then, this gear was coupled with other no-grounded gear of the same kind (but without motor). The simulator was configured for 1000 frames, with 200 steps per frame at 300°K. This design (Figure 9) has 340 atoms and 0 grounds

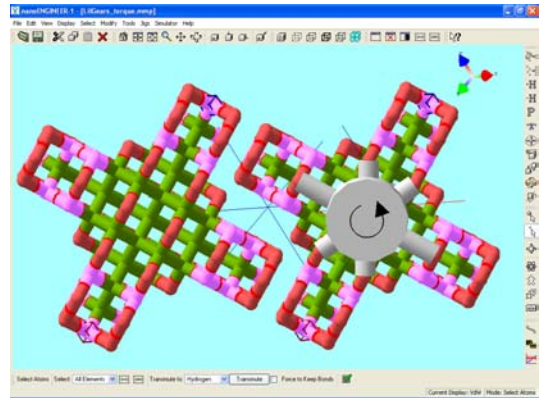
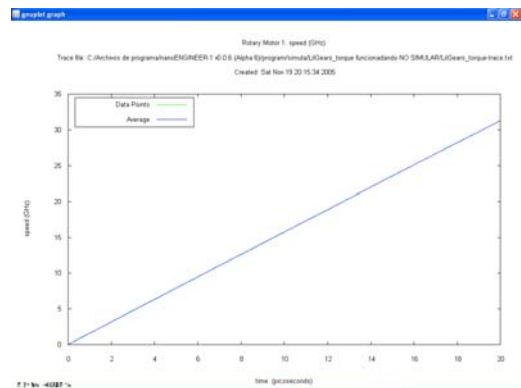
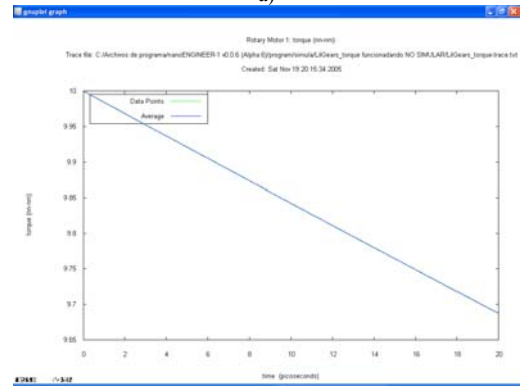


Figure 9. A pair of coupled gears in Lines display mode

The simulation results (video) show that the gear turns a half time. Figure 10a, shows the rotation speed of the motor growing lineally; it shows that in 20ps it achieves approximately 32GHz. Figure 10b shows the torque exerted by the motor and Figure 11 shows a video image that allows to know that if a no-grounded structure is hit by other (in this case the hit is caused by the rotary gear), it is shifted.



a)



b)

Figure 10. Graphical simulation results of the LilGears Variation with two gear. a) Speed, b) Torque.

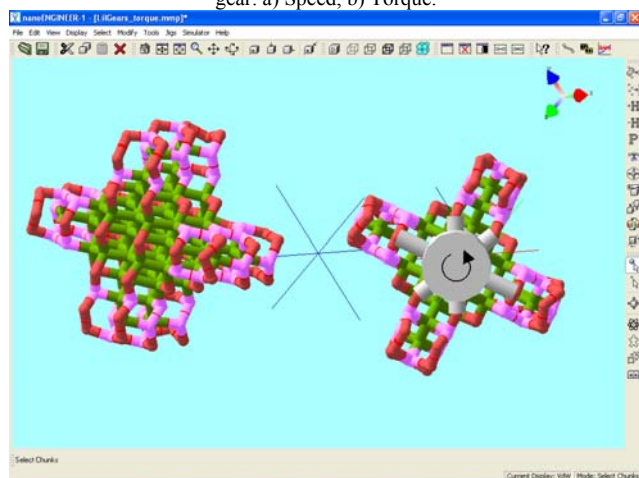


Figure 11. A Video image showing the result of simulate collision of a no-ground design

6.3 Carbon Nanotube and Benzene Gear.

This gear designed is a variation of the proposed in [12]. It consists in a pair of carbon nanotubes with 7 benzene teeth. In this case (Figure 12), a motor is attached to one of them and it is supposed that the other will turn by the interaction with the first. They are made of H and C. The motor was configured using the following parameters: torque 0.1nN-nm, speed 1 GHz, length 5 Å, radio 1 Å, and spoke radio 0.5 Å. The simulator was programmed to 600 frames, with 10 steps per frame at 300°K. This design has 364 atoms and 0 grounds.

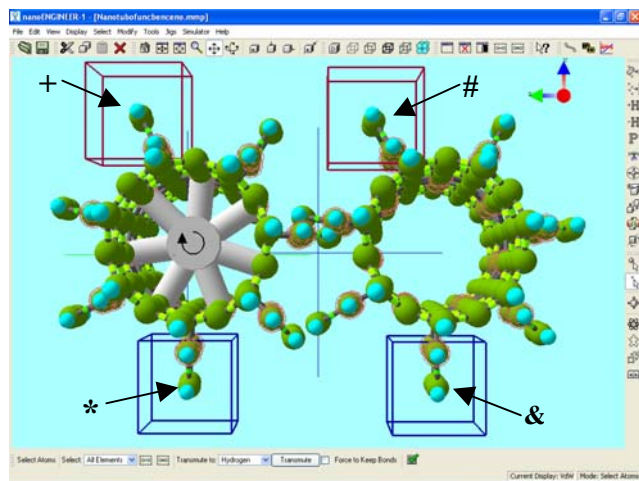
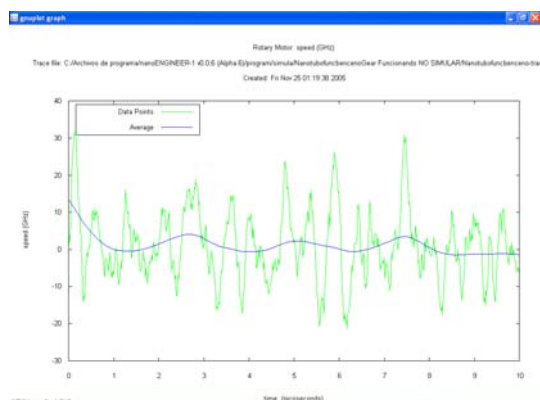


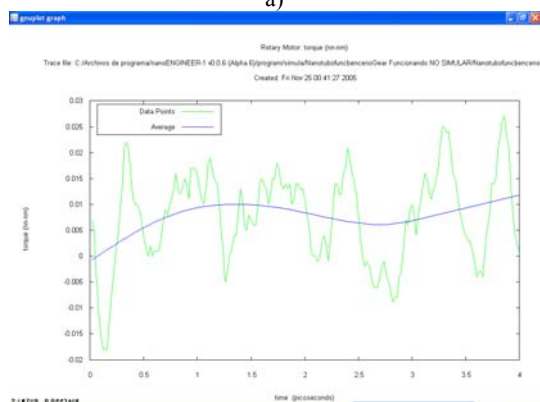
Figure 12. Carbon Nanotube and Benzene Gear in CPK display mode

The simulation results (video) show that the gear does not turn. Figure 13a, shows that the rotation speed of the motor shows a abnormal behavior, in average is like a sinusoidal, the maximum is 12GHz and the minimum is -1GHz (the minus is according to the direction). Figure 13b shows the torque exerted by the motor, also with a

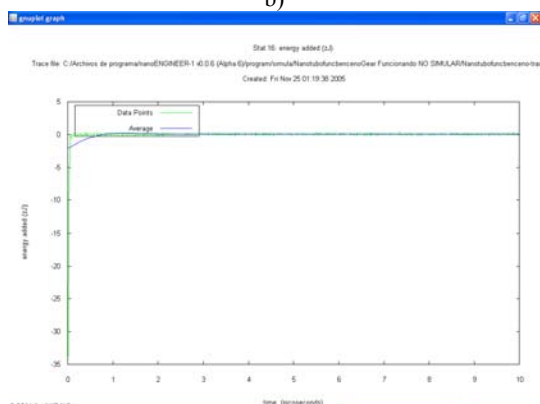
abnormal behavior. It is important to mention that in this case the torque does not present the complementary behavior of the motor, similar to the other cases. Figure 13c shows the energy added to the atom identified by * in Figure 12 to the gear with motor, Figure 13d shows the temperature measured on the atom identified by + in Figure 12, both are approximately constant, with a pick at the beginning. It is important to take care of the pick in the temperature that is about 3300 ° K, due it could cause the damage of a near structure, including the damage of it. Figure 13e shows the energy added to the atom identified by & in Figure 12 to the gear without motor. Figure 13f shows the temperature measured on the atom identified by # in Figure 12.



a)



b)



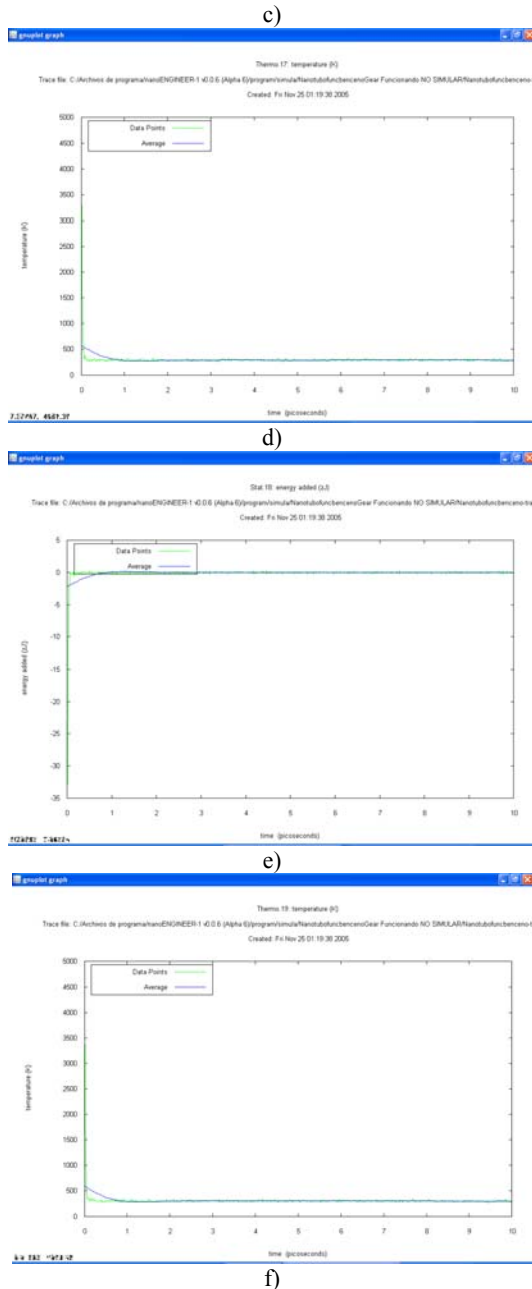


Figure 13. Graphical simulation results of the Carbon-Benzene Gear. a) Speed, b) Torque, c) Energy added, d) Temperature to the Gear with motor, e) Energy added, f) Temperature to the Gear without motor

6.4 MarkIII [k] Planetary Gear.

It is made of H, C, O, Si, N, S, P. The motor was configured using the following parameters: torque 10nN-nm, speed 1000 GHz (1 THz), length 10 Å, radius 2 Å, and spoke radius 0.5 Å. The simulator was configured for 1000 frames, with 200 steps per frame at 300°K. This design (Figure 14) has 3853 atoms and 5 Grounds

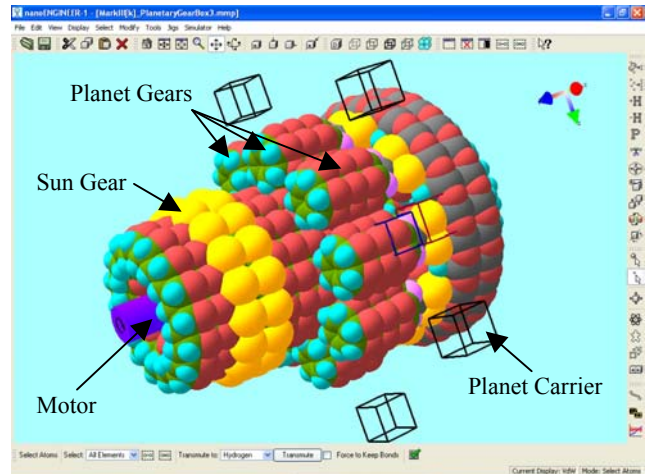
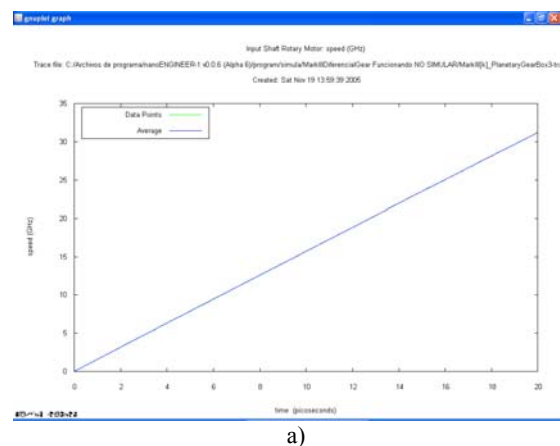
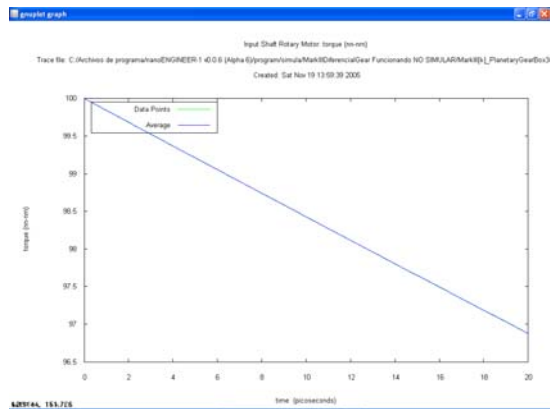


Figure 14. MarkIII [k] Planetary Gear without casing (the black boxes are ground attachments) in VdW display mode

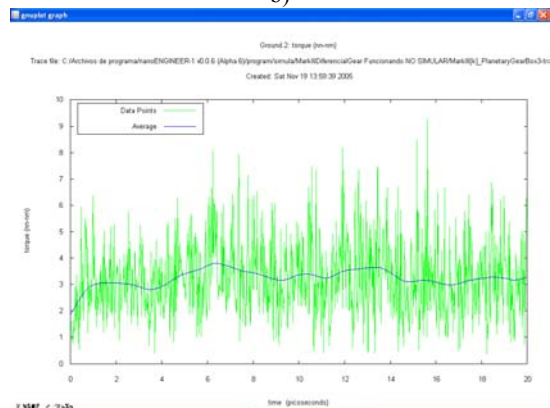
The Mark III Planetary Gear is a planetary gear created by K. Eric Drexler. A planetary gear couples an input shaft via a sun gear to an output shaft through a set of planet gears (attached to the output shaft by a planet carrier). The planet gears roll between the sun gear and a ring gear on the inner surface of a casing giving a Gear of Ratio: 45:16 and a Speed Ratio: 2.8125:1. Planetary gears are common mechanical systems used for speed reduction (= torque multiplication). Macroscale versions are found in automobile transmissions, electric screwdrivers, and Mars Landers [13].

The simulation results (video) show that the gear turns $\frac{1}{4}$ of turn. Figure 15a, shows the rotation speed of the motor growing lineally; it shows that in 20ps it achieves approximately 32GHz. Figure 15b shows the torque exerted by the motor and Figure 15c shows the torque exerted in the ground.





b)



c)

Figure 15. Graphical simulation results of the MarkIII [k] Differential Gear. a) Speed, b) Torque, c) Torque at the Ground

6.5 Drexler-Merkle Differential Gear.

It is made of H, C, O, Si, S, P. The motor was configured using the following parameters: torque 100nN-nm, speed 1000GHz (1 THz), length 10 Å, radius 2 Å, and spoke radius 0.5 Å. The simulator was configured for 1000 frames, with 200 steps per frame at 300°K. This design (Figure 16) has 8292 atoms and 8 Grounds (the blue cube is a thermostat at 306°K)

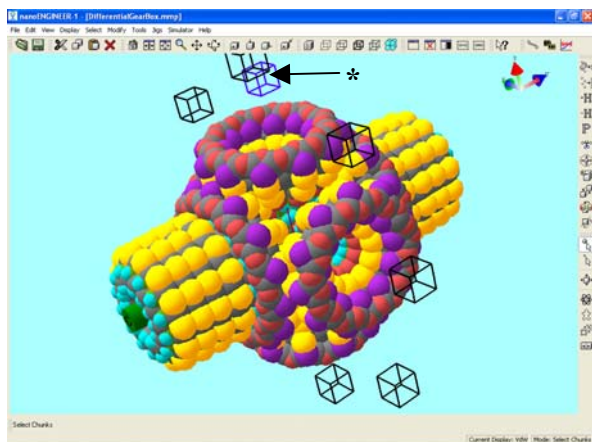
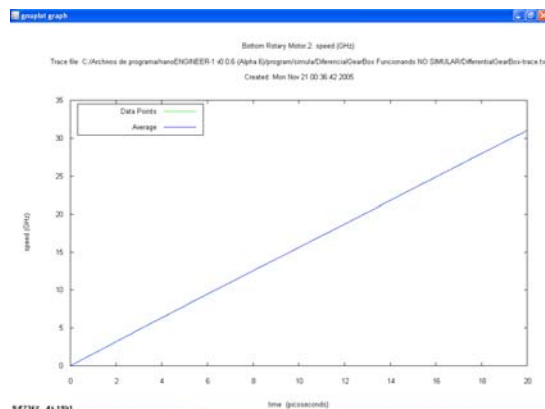
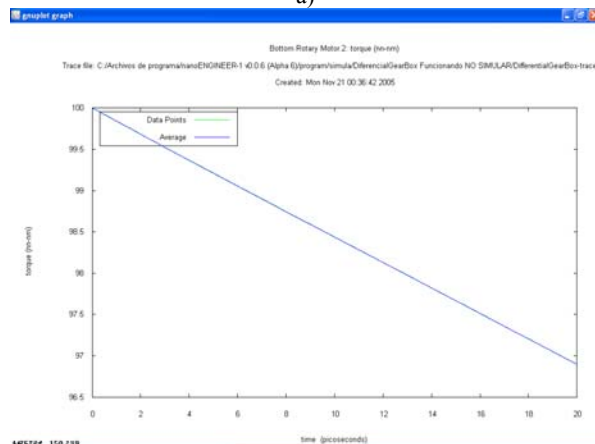


Figure 16. Drexler-Merkle Differential Gear without casing (the black boxes are ground attachments) in VdW display mode

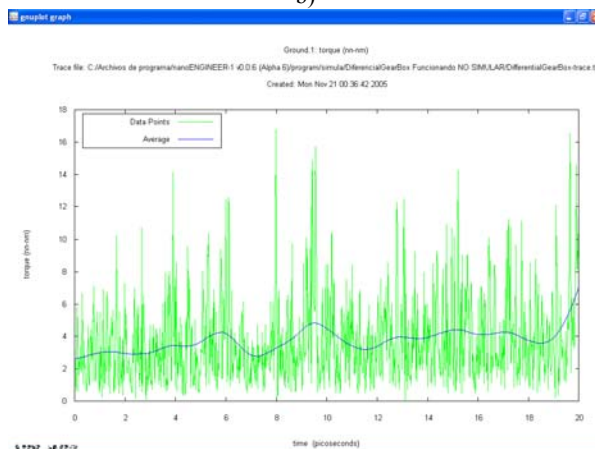
The simulation results (video) show that the gear turns ¼ of turn. Figure 17a, shows the rotation speed of the motor growing lineally; it shows that in 20ps it achieves approximately 32GHz. Figure 17b shows the torque exerted by the motor and Figure 17c shows the torque exerted in the ground, which has an abnormal behavior, that could be caused by the vibration and interaction of the 5 movil parts of the gear and Figure 17d shows the energy added to the atom identified by * in Figure 16.



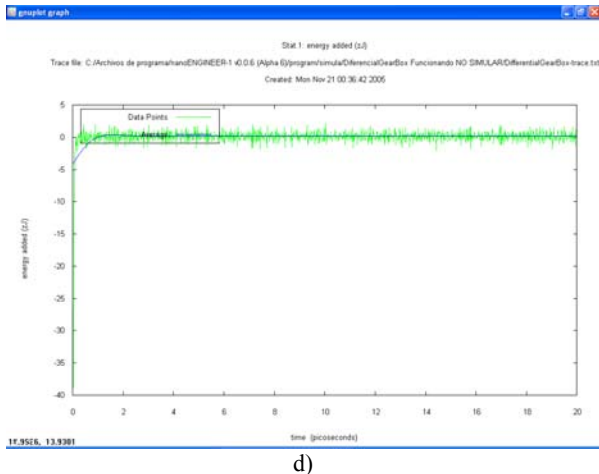
a)



b)



c)



d)
Figure 17. Graphical simulation results of the MarkIII [k] Differential Gear. a) Speed, b) Torque, c) Torque at the Ground, d)Energy added

7. CONCLUSIONS AND FUTURE WORK

This work shows that nanoengineer-1 is very suitable to design nanomachines on a personal computer.

The methodology proposed allows to design nanostructures of medium complexity, which could be putted together with others, to design complex nanomachines.

The Nanomechanical simulation carried out using nanoengineer-1, allows to make an analysis of the structure and of the dynamical behavior of the design.

The simulations presented in this work were carried out in order to understand the concepts of the nanomachines with the purpose of designing nanorobots and nanofactories, for biomedical and spatial applications, and nanodevices for computation tasks.

The future work is oriented to analyze some nanoscale events presented during simulation and compare the simulation results with theoretic results.

6. REFERENCES

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